



# STIC Search Report

## Biotech-Chem Library

STIC Database Tracking Number: 155417

TO: Tamthom Troung

Location: REM/5C18

Art Unit: 1624

June 23, 2005

Case Serial Number: 10/725657

From: P. Sheppard

Location: Remsen Building

Phone: (571) 272-2529

sheppard@uspto.gov

### Search Notes

=> fil hcaplus  
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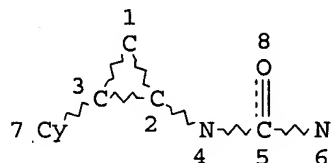
FILE COVERS 1907 - 23 Jun 2005 VOL 142 ISS 26  
 FILE LAST UPDATED: 22 Jun 2005 (20050622/ED)

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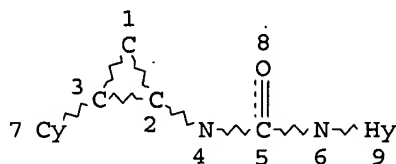
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 NUMBER OF NODES IS 8

STEREO ATTRIBUTES: NONE  
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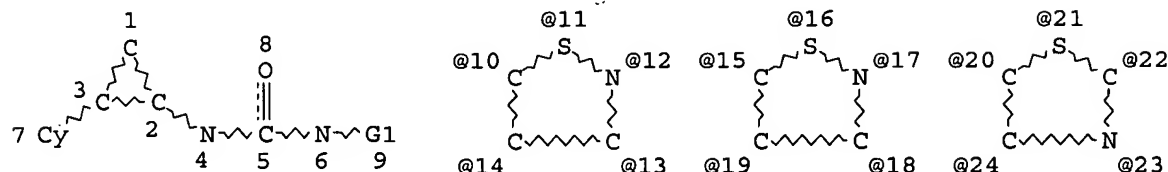
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GRAPH ATTRIBUTES:

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NUMBER OF NODES IS 24

STEREO ATTRIBUTES: NONE

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L14 ANSWER 1 OF 1 HCAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 1972:547456 HCAPLUS

DOCUMENT NUMBER: 77:147456

TITLE: 1-Alkyl-3-(3-alkyl-5-nitro-4-thiazolin-2-ylidene)ureas and related compounds as schistosomicides

AUTHOR(S): Werbel, Leslie M.; Degnan, Margaret B.; Harger, Gail F.; Capps, David B.; Islip, Peter J.; Closier, Michael D.

CORPORATE SOURCE: Res. Dev. Div., Parke, Davis and Co., Ann Arbor, MI, USA

SOURCE: Journal of Medicinal Chemistry (1972), 15(9), 955-63  
CODEN: JMCMAR; ISSN: 0022-2623

DOCUMENT TYPE: Journal

LANGUAGE: English

AB Many 1-alkyl-3-[3-(alkyl or aralkyl)-5-nitro-4-thiazolin-2-ylidene]ureas (analogues of niridazole) were curative against *Schistosoma mansoni* in mice, and several were curative in rhesus monkeys but not tolerated by dogs. Among the most active compds. tested was 1-ethyl-3-(3-benzyl-5-nitro-4-thiazoline-2-ylidene)urea (I) [26231-01-6], which was curative at 100 mg/kg/day for 5 days by gavage in mice and at a similar dosage in monkeys. Structure-activity relations were discussed. To synthesize I,

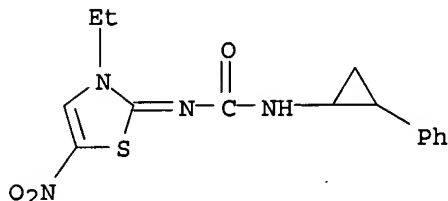
2-amino-5-nitrothiazole was reacted with EtNCO to form  
1-ethyl-3-(5-nitro-2-thiazolyl)urea, which was then reacted with BzI in  
the presence of NaH.

IT 38908-70-2

RL: BAC (Biological activity or effector, except adverse); BSU (Biological  
study, unclassified); BIOL (Biological study)  
(schistosomicidal activity of)

RN 38908-70-2 HCAPLUS

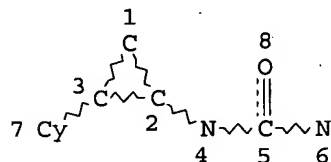
CN Urea, (3-ethyl-5-nitro-2(3H)-thiazolylidene)(2-phenylcyclopropyl)- (9CI)  
(CA INDEX NAME)



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L1 STR



NODE ATTRIBUTES:

DEFAULT MLEVEL IS ATOM

DEFAULT ECLEVEL IS LIMITED

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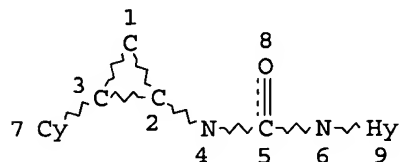
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NUMBER OF NODES IS 8

STEREO ATTRIBUTES: NONE

L3 509 SEA FILE=REGISTRY SSS FUL L1

L4 STR



NODE ATTRIBUTES:

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DEFAULT ECLEVEL IS LIMITED

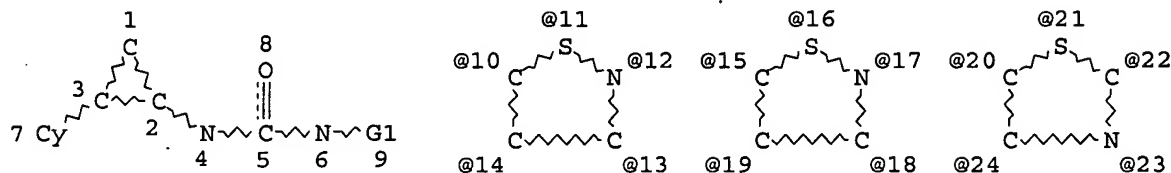
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NUMBER OF NODES IS 9

STEREO ATTRIBUTES: NONE

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DEFAULT ECLEVEL IS LIMITED

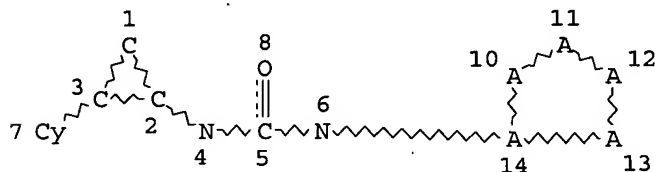
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NUMBER OF NODES IS 24

STEREO ATTRIBUTES: NONE

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L12 STR



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DEFAULT MLEVEL IS ATOM

DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:

RING(S) ARE ISOLATED OR EMBEDDED

NUMBER OF NODES IS 13

STEREO ATTRIBUTES: NONE

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L16 5 SEA FILE=HCAPLUS ABB=ON PLU=ON L15  
L17 5 SEA FILE=HCAPLUS ABB=ON PLU=ON L16 NOT L14

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L17 ANSWER 1 OF 5 HCAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 2004:902086 HCAPLUS

DOCUMENT NUMBER: 141:388753

TITLE: Heterocyclic compound modulators of Tie-2 and other kinases, and therapeutic use

INVENTOR(S): Chen, Jeff; Dalrymple, Lisa; Epshteyn, Sergey;

Forsyth, Timothy; Huynh, Tai; Leahy, James; Mann, Grace; Mann, Larry W.; Ridgway, Brian; Sangalang, Joan C.; Takeuchi, Craig  
 PATENT ASSIGNEE(S): Exelixis, Inc., USA  
 SOURCE: PCT Int. Appl., 126 pp.  
 CODEN: PIXXD2  
 DOCUMENT TYPE: Patent  
 LANGUAGE: English  
 FAMILY ACC. NUM. COUNT: 1  
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2004091480	A2	20041028	WO 2004-US10626	20040408
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, GR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW RW: BW, GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				

PRIORITY APPLN. INFO.: US 2003-461471P P 20030409

OTHER SOURCE(S): MARPAT 141:388753

AB The invention provides heterocyclic compds. for modulating protein kinase enzymic activity for modulating cellular activities such as proliferation, differentiation, programmed cell death, migration and chemoinvasion. Compds. of the invention inhibit, regulate and/or modulate kinases, particularly Tie-2. Methods of using the compds. and pharmaceutical compns. thereof to treat kinase-dependent diseases and conditions are also an aspect of the invention. Preparation of triazolyl compds. of the invention is included.

IT 783327-32-2

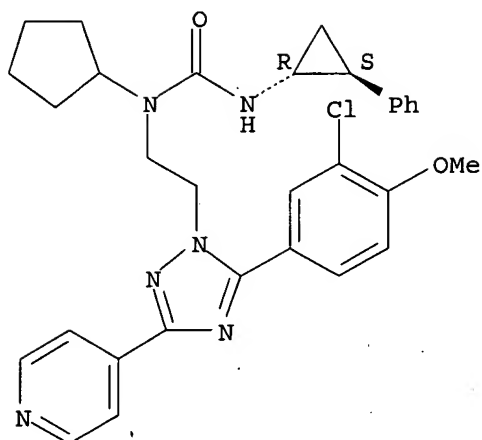
RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); USES (Uses)

(heterocyclic compound modulators of Tie-2 and other kinases, and therapeutic use)

RN 783327-32-2 HCAPLUS

CN Urea, N-[2-[5-(3-chloro-4-methoxyphenyl)-3-(4-pyridinyl)-1H-1,2,4-triazol-1-yl]ethyl]-N-cyclopentyl-N'-[(1R,2S)-2-phenylcyclopropyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L17 ANSWER 2 OF 5 HCAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 2004:780696 HCAPLUS

DOCUMENT NUMBER: 141:295849

TITLE: Preparation of carboxamidopyrrolidines as melanin-concentrating hormone receptor antagonists and compositions and methods related thereto

INVENTOR(S): Goodfellow, Val; Rowbottom, Martin; Dyck, Brian P.; Tamiya, Junko; Zhang, Mingzhu; Grey, Jonathan; Vickers, Troy D.

PATENT ASSIGNEE(S): Neurocrine Biosciences, Inc., USA

SOURCE: PCT Int. Appl., 180 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2004081005	A1	20040923	WO 2004-US7259	20040308
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RW:	BW, GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG			

PRIORITY APPLN. INFO.: US 2003-452776P P 20030307  
US 2003-518265P P 20031107

OTHER SOURCE(S): MARPAT 141:295849

GI

\* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT \*

AB Title compds. I [m = 0 or 1; n = 1 or 2; X = -CH<sub>2</sub>-, or -N(R<sub>6</sub>)-; R<sub>1</sub> = H, (un)substituted-alkyl, -aryl, -arylalkyl, etc.; R<sub>2</sub> and R<sub>5</sub> independently = H, (un)substituted alkyl; R<sub>3</sub> = H, (un)substituted-alkyl, -arylalkyl, -heteroarylalkyl; R<sub>4</sub> = (un)substituted-alkyl, -aryl, -heterocycle; R<sub>6</sub> = H or (un)substituted alkyl] and their pharmaceutically acceptable salt, are disclosed as melanin-concentrating hormone (MCH) receptor antagonists having utility for the treatment of MCH receptor-based disorders such as obesity. Thus, e.g., II was prepared via amidation of of III (preparation given) with benzoyl chloride. Methods for evaluation of compds. are described (no data). Also disclosed are compns. containing a compound of this invention, as well as methods relating to the use thereof.

IT 762278-96-6P 762279-03-8P 762279-04-9P  
762279-05-0P 762279-06-1P 762284-01-5P  
762284-02-6P 762284-03-7P 763130-70-7P  
763131-31-3P 763131-32-4P

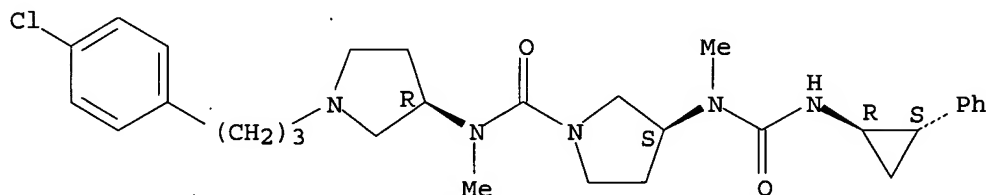
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(drug candidate; preparation of carboxamidopyrrolidine derivs. as melanin-concentrating hormone receptor antagonists)

RN 762278-96-6 HCAPLUS

CN 1-Pyrrolidinecarboxamide, N-[(3R)-1-[3-(4-chlorophenyl)propyl]-3-pyrrolidinyl]-N-methyl-3-[methyl[[[(1R,2S)-2-phenylcyclopropyl]amino]carbonyl]amino]-, (3S)- (9CI) (CA INDEX NAME)

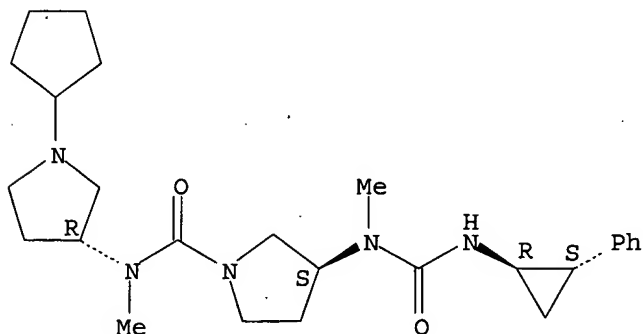
Absolute stereochemistry.



RN 762279-03-8 HCAPLUS

CN 1-Pyrrolidinecarboxamide, N-[(3R)-1-cyclopentyl-3-pyrrolidinyl]-N-methyl-3-[methyl[[[(1R,2S)-2-phenylcyclopropyl]amino]carbonyl]amino]-, (3S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



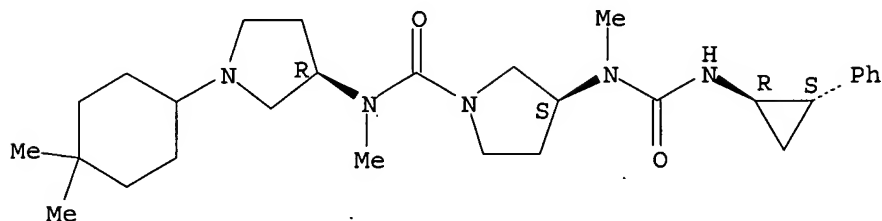
RN 762279-04-9 HCAPLUS

CN 1-Pyrrolidinecarboxamide, N-[(3R)-1-(4,4-dimethylcyclohexyl)-3-



pyrrolidinyl]-N-methyl-3-[methyl[[[(1R,2S)-2-phenylcyclopropyl]amino]carbonyl]amino]-, (3S)- (9CI) (CA INDEX NAME)

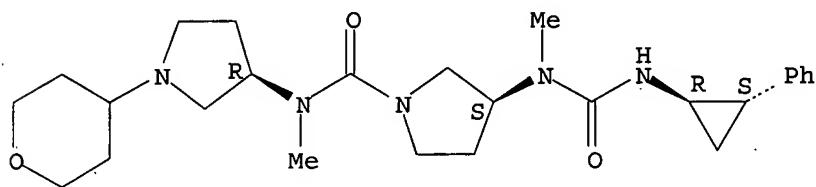
Absolute stereochemistry.



RN 762279-05-0 HCAPLUS

CN 1-Pyrrolidinecarboxamide, N-methyl-3-[methyl[[[(1R,2S)-2-phenylcyclopropyl]amino]carbonyl]amino]-N-[(3R)-1-(tetrahydro-2H-pyran-4-yl)-3-pyrrolidinyl]-, (3S)- (9CI) (CA INDEX NAME)

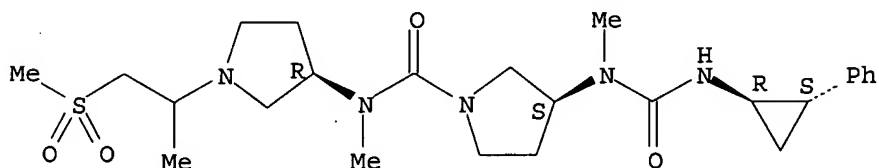
Absolute stereochemistry.



RN 762279-06-1 HCAPLUS

CN 1-Pyrrolidinecarboxamide, N-methyl-N-[(3R)-1-[1-methyl-2-(methylsulfonyl)ethyl]-3-pyrrolidinyl]-3-[methyl[[[(1R,2S)-2-phenylcyclopropyl]amino]carbonyl]amino]-, (3S)- (9CI) (CA INDEX NAME)

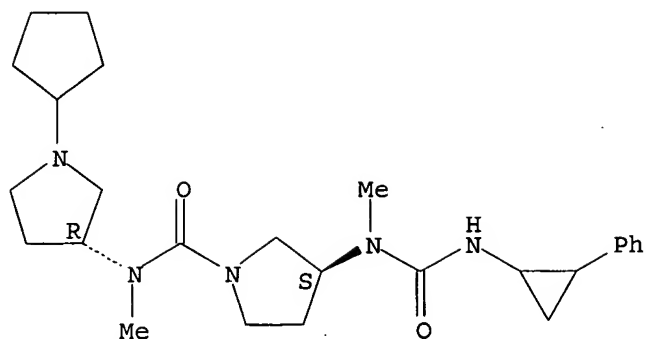
Absolute stereochemistry.



RN 762284-01-5 HCAPLUS

CN 1-Pyrrolidinecarboxamide, N-[(3R)-1-cyclopentyl-3-pyrrolidinyl]-N-methyl-3-[methyl[[[(2-phenylcyclopropyl)amino]carbonyl]amino]-, (3S)- (9CI) (CA INDEX NAME)

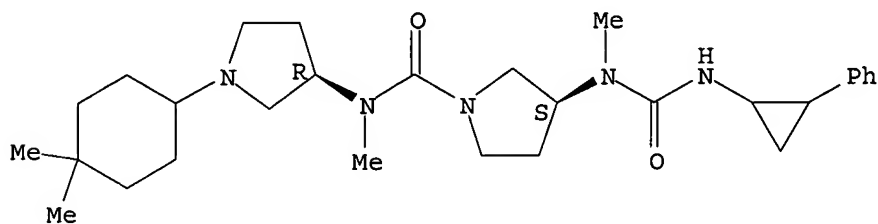
Absolute stereochemistry.



RN 762284-02-6 HCAPLUS

CN 1-Pyrrolidinecarboxamide, N-[(3R)-1-(4,4-dimethylcyclohexyl)-3-pyrrolidinyl]-N-methyl-3-[methyl[(2-phenylcyclopropyl)amino]carbonyl]amino]-, (3S)- (9CI) (CA INDEX NAME)

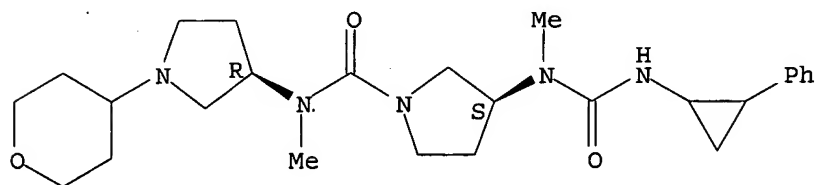
Absolute stereochemistry.



RN 762284-03-7 HCAPLUS

CN 1-Pyrrolidinecarboxamide, N-methyl-3-[methyl[(2-phenylcyclopropyl)amino]carbonyl]amino]-N-[(3R)-1-(tetrahydro-2H-pyran-4-yl)-3-pyrrolidinyl]-, (3S)- (9CI) (CA INDEX NAME)

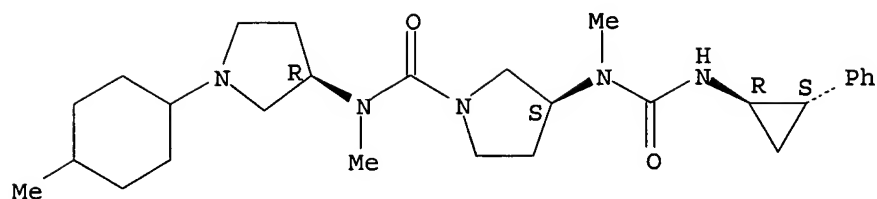
Absolute stereochemistry.



RN 763130-70-7 HCAPLUS

CN 1-Pyrrolidinecarboxamide, N-methyl-N-[(3R)-1-(4-methylcyclohexyl)-3-pyrrolidinyl]-3-[methyl[[[(1R,2S)-2-phenylcyclopropyl]amino]carbonyl]amino]-, (3S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 763131-31-3 HCAPLUS

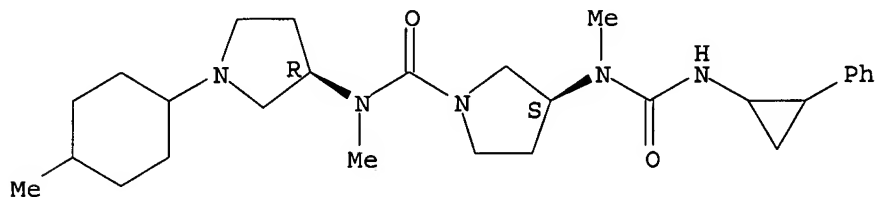
CN 1-Pyrrolidinecarboxamide, N-methyl-N-[(3R)-1-(4-methylcyclohexyl)-3-pyrrolidinyl]-3-[methyl[(2-phenylcyclopropyl)amino]carbonyl]amino]-, (3S)-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

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CRN 763131-30-2

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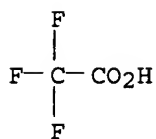
Absolute stereochemistry.



CM 2

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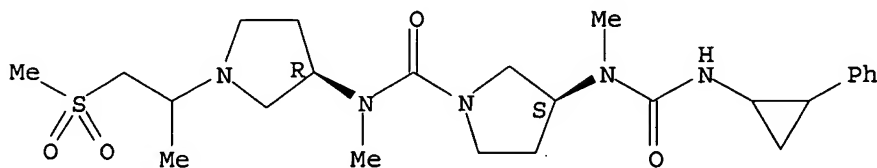
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RN 763131-32-4 HCAPLUS

CN 1-Pyrrolidinecarboxamide, N-methyl-N-[(3R)-1-[1-methyl-2-(methylsulfonyl)ethyl]-3-pyrrolidinyl]-3-[methyl[(2-phenylcyclopropyl)amino]carbonyl]amino]-, (3S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



REFERENCE COUNT: 4 THERE ARE 4 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L17 ANSWER 3 OF 5 HCAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 2003:591157 HCAPLUS

DOCUMENT NUMBER: 139:149641

TITLE: Preparation of pyrimidinones as viral polymerase inhibitors

INVENTOR(S): Avolio, Salvatore; Colarusso, Stefania; Conte, Immacolata; Harper, Steven; Koch, Uwe; Malancona, Savina; Matassa, Victor Giulio; Narjes, Frank; Petrocchi, Alessia; Summa, Vincenzo

PATENT ASSIGNEE(S): Istituto Di Ricerche Di Biologia Molecolare P. Angeletti Spa, Italy

SOURCE: PCT Int. Appl., 82 pp.

CODEN: PIXXD2

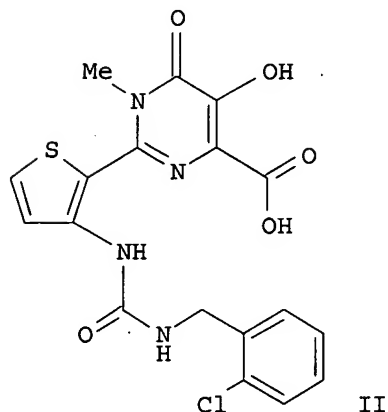
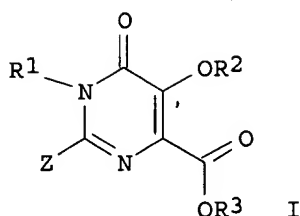
DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2003062211	A1	20030731	WO 2003-GB124	20030115
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RW:	GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG			
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EP 1470113	A1	20041027	EP 2003-700366	20030115
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US 2005130997	A1	20050616	US 2003-500971	20030115
PRIORITY APPLN. INFO.:			GB 2002-1179	A 20020118
			WO 2003-GB124	W 20030115
OTHER SOURCE(S):	MARPAT 139:149641			
GI				



AB Title compds. I [wherein Z = (un)substituted alkynyl, aryl, or heteroaryl; R1 = (un)substituted alkyl or (aryl)alkyl; R2 = H, (un)substituted alkyl, alkylcarbonyl, aryl, arylcarbonyl, heteroaryl, (aryl)alkyl, (heteroaryl)alkyl; R3 = H, alkyl, (heterocycloalkyl)alkyl, dialkylaminoalkyl, (alkylcarbonyloxy)alkyl, (cycloalkoxycarbonyloxy)alkyl; and their pharmaceutically acceptable salts] were prepared as inhibitors of viral polymerases, especially the hepatitis C virus (HCV) polymerase enzyme. For example, II was prepared from 3-nitrothiophene-2-carbonitrile (preparation given) by base-catalyzed nucleophilic addition of hydroxylamine, reaction with di-Me acetylenedicarboxylate in CH<sub>2</sub>Cl<sub>2</sub>, intramol. cyclocondensation in xylene, room temperature O-acylation with pivaloyl chloride in the presence of 4-DMAP, base-catalyzed N-methylation with di-Me sulfate for 1 h, hydrogenation over Pd/C, and reaction with ortho-chlorobenzyl isocyanate in dichloromethane. I exhibited an IC<sub>50</sub> value of 100  $\mu$ M or less for inhibition of HCV polymerase. Thus, I and their pharmaceutical compns. are useful for treating or preventing an illness due to HCV (no data).

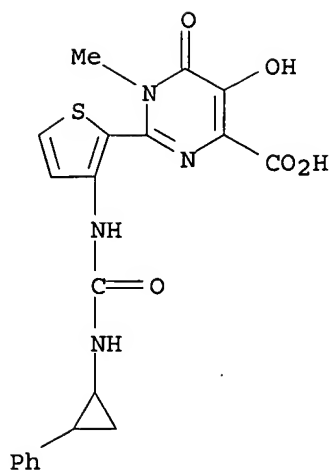
IT 572917-01-2P

RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(viral polymerase inhibitor; preparation of pyrimidinones as viral polymerase inhibitors)

RN 572917-01-2 HCAPLUS

CN 4-Pyrimidinecarboxylic acid, 1,6-dihydro-5-hydroxy-1-methyl-6-oxo-2-[3-[[[(2-phenylcyclopropyl)amino]carbonyl]amino]-2-thienyl]- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 3 THERE ARE 3 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L17 ANSWER 4 OF 5 HCAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 2002:465982 HCAPLUS

DOCUMENT NUMBER: 137:47213

TITLE: Preparation of fused pyrimidinones and benzodioxaborolidinylpropylaminopyrrolo[1,2-a]pyrimidines as inhibitors of hepatitis C ns3 protease for the treatment of hepatitis C and other viral diseases

INVENTOR(S): Glunz, Peter W.; Douty, Brent D.; Han, Wei

PATENT ASSIGNEE(S): Bristol-Myers Squibb Pharma Company, USA

SOURCE: PCT Int. Appl., 270 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2002048116	A2	20020620	WO 2001-US47911	20011212
W:	AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PH, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM			
RW:	GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG			
AU 2002030763	A5	20020624	AU 2002-30763	20011212
US 2003064962	A1	20030403	US 2001-15304	20011212
US 6653295	B2	20031125		

PRIORITY APPLN. INFO.: US 2000-255290P P 20001213  
WO 2001-US47911 W 20011212

OTHER SOURCE(S): MARPAT 137:47213

GI

\* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT \*

AB Fused pyrimidinones I [A1 = (un)substituted CH<sub>2</sub>, CH<sub>2</sub>CH<sub>2</sub>, CH<sub>2</sub>CH<sub>2</sub>CH<sub>2</sub>, A2CH<sub>2</sub>, A2CH<sub>2</sub>CH<sub>2</sub>, CH<sub>2</sub>A2CH<sub>2</sub>; A2 = O, S, (un)substituted imino; A3 = H, R<sub>9</sub>CO, R<sub>9</sub>O, R<sub>9</sub>S, R<sub>9</sub>CONH, R<sub>9</sub>NHCO, etc.; W = (un)substituted boronic acid ester; QCOCO, QNHCOCO, QOCOCO, QNHCOCF<sub>2</sub>CO, COQ3, F3CCO, F3CCF<sub>2</sub>CO, OHC, amino acid residue; Q3 = (un)substituted aryl, heterocyclyl; R1 = H, F, (un)substituted alkyl, alkenyl, alkynyl, cycloalkyl; R2 = H, alkyl; Q, R3, R9 = (un)substituted alkyl, alkenyl, alkynyl, cycloalkyl, aryl, heterocyclyl; R6, R13 = H, (un)substituted alkyl, alkenyl, alkynyl, cycloalkyl, aryl, aralkyl, cycloalkylalkyl; R3R13 = (un)substituted carbocyclic ring, alkylidene] and particularly dioxaborolylpropylamino pyrrolopyriminecarboxamides such as II are prepared as inhibitors of hepatitis C viral protein ns3 protease for the treatment of hepatitis C and other viral diseases. E.g., esterification of L-pyrogutamic acid with AcOCMe<sub>3</sub> and HClO<sub>4</sub>, thionation with Lawesson's reagent, S-methylation with MeI, and amidation with NH<sub>4</sub>Cl gives nonracemic aminopyrrolinecarboxylate III. Treatment of III with di-Me 2-(methoxymethylene)malonate, hydrolysis of the Me ester moiety with LiOH, preparation of the acyl azide with diphenylphosphoryl azide and Curtius rearrangement in the presence of PhCH<sub>2</sub>OH, and hydrolysis of the tert-Bu ester with CF<sub>3</sub>CO<sub>2</sub>H gives pyrrolo[1,2-a]pyrimidine IV. Coupling of IV with an α-allyl aminomethylboronate pinanediol ester gives II. I inhibit hepatitis C ns3 protease with IC<sub>50</sub> values of <100 μM. Pharmaceutical compns. containing I are given.

IT 437758-67-3P 437758-68-4P

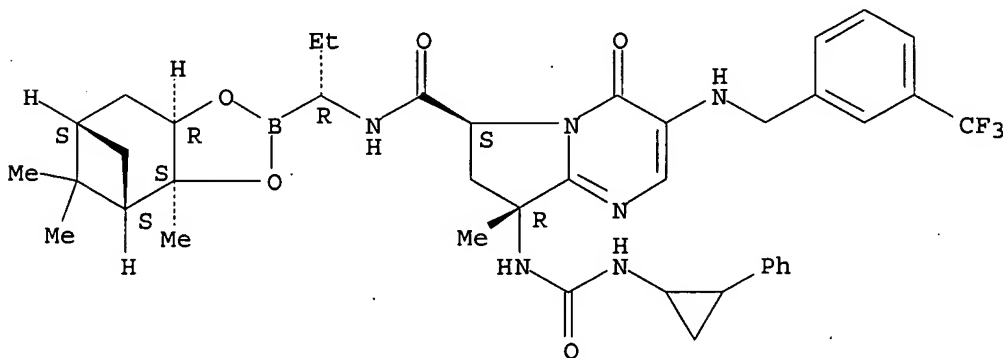
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(invention compd; preparation of fused pyrimidinones and benzodioxaborolidinylpropylaminopyrrolo[1,2-a]pyrimidines as inhibitors of hepatitis C ns3 protease for the treatment of hepatitis C and other viral diseases)

RN 437758-67-3 HCAPLUS

CN Pyrrolo[1,2-a]pyrimidine-6-carboxamide, N-[(1R)-1-[(3aS,4S,6S,7aR)-hexahydro-3a,5,5-trimethyl-4,6-methano-1,3,2-benzodioxaborol-2-yl]propyl]-4,6,7,8-tetrahydro-8-methyl-4-oxo-8-[[[(2-phenylcyclopropyl)amino]carbonylamino]-3-[[[3-(trifluoromethyl)phenyl]methyl]amino]-, (6S,8R)-(9CI) (CA INDEX NAME)

Absolute stereochemistry.

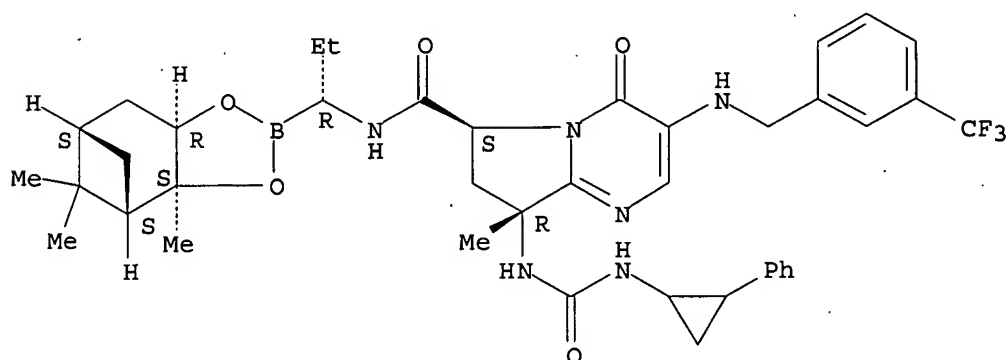


RN 437758-68-4 HCAPLUS  
 CN Pyrrolo[1,2-a]pyrimidine-6-carboxamide, N-[(1R)-1-[(3aS,4S,6S,7aR)-hexahydro-3a,5,5-trimethyl-4,6-methano-1,3,2-benzodioxaborol-2-yl]propyl]-4,6,7,8-tetrahydro-8-methyl-4-oxo-8-[[[(2-phenylcyclopropyl)amino]carbonyl]amino]-3-[[[3-(trifluoromethyl)phenyl]methyl]amino]-, (6S,8R)-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

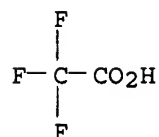
CRN 437758-67-3  
 CMF C40 H48 B F3 N6 O5

Absolute stereochemistry.



CM 2

CRN 76-05-1  
 CMF C2 H F3 O2

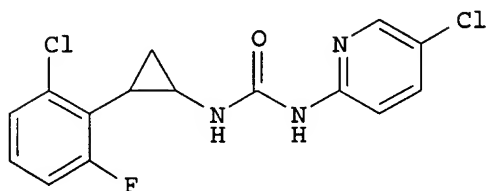


L17 ANSWER 5 OF 5 HCAPLUS COPYRIGHT 2005 ACS on STN  
 ACCESSION NUMBER: 1995:789162 HCAPLUS  
 DOCUMENT NUMBER: 123:198634  
 TITLE: Preparation of N-[aryl(cyclo)alkyl]-N'-pyridylureas and analogs as HIV reverse transcriptase inhibitors  
 INVENTOR(S): Lind, Peter Thomas; Noreen, Rolf; Morin, John Michael; Ternansky, Robert John  
 PATENT ASSIGNEE(S): Medivir AB, Swed.  
 SOURCE: PCT Int. Appl., 104 pp.  
 CODEN: PIXXD2  
 DOCUMENT TYPE: Patent  
 LANGUAGE: English  
 FAMILY ACC. NUM. COUNT: 1  
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
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WO 9506034	A1	19950302	WO 1994-US9406	19940824
W: AT, AU, BB, BG, BR, BY, CA, CH, CN, CZ, DE, DK, ES, FI, GB, HU, JP, KP, KR, KZ, LK, LU, LV, MG, MN, MW, NL, NO, NZ, PL, PT, RO, RU, SD, SE, SK, UA, US, UZ, VN				
RW: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, ML, MR, NE, SN, TD, TG				
CA 2168447	AA	19950302	CA 1994-2168447	19940824
AU 9477153	A1	19950321	AU 1994-77153	19940824
AU 687440	B2	19980226		
EP 706514	A1	19960417	EP 1994-927932	19940824
EP 706514	B1	19981118		
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LI, LU, NL, PT, SE				
JP 09502702	T2	19970318	JP 1994-507689	19940824
AT 173466	E	19981215	AT 1994-927932	19940824
ES 2123156	T3	19990101	ES 1994-927932	19940824
NZ 273741	A	20000623	NZ 1994-273741	19940824
US 5849769	A	19981215	US 1996-601030	19960503
US 6376492	B1	20020423	US 2000-567857	20000509
US 2002132794	A1	20020919	US 2002-76163	20020213
US 2004116418	A1	20040617	US 2003-725657	20031201
PRIORITY APPLN. INFO.:			US 1993-110956	A 19930824
			WO 1994-US9406	W 19940824
			US 1996-601030	A3 19960503
			US 1998-114935	B1 19980714
			US 2000-567857	A3 20000509
			US 2002-76163	A3 20020213
OTHER SOURCE(S):			MARPAT 123:198634	
GI				



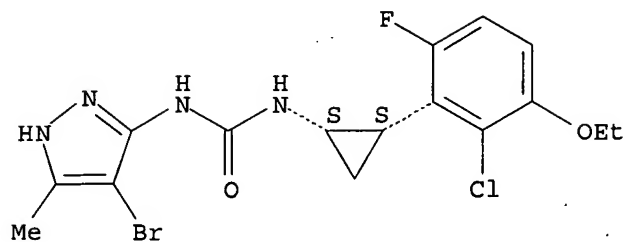
AB R2R4NZNR1R3 [R1 = (heterocyclic) organic ring residue; R2 = CR7R9CR5R6R8; R3,R4 = H, OH, alk(en)yl, CONH2, etc.; R5 = groups cited for R1, NH2, OH, alkoxy, etc.; R6-R9 = H, (cyclo)alkyl, halo, NH2, CO2H, etc.; Z = CO, C(:NH), C(:CH2), SO2, etc.] were prepared Thus, cis-2-(2-chloro-6-fluorophenyl)cyclopropylisocyanate (preparation from 2-chloro-6-fluorobenzaldehyde given) was condensed with 2-amino-5-chloropyridine to give title compound cis-I which had IC50 of 0.0004µg/mL against HIV reverse transcriptase in vitro.

IT 167683-23-0P  
 RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)  
 (preparation of N-[aryl(cyclo)alkyl]-N'-pyridylureas and analogs as HIV reverse transcriptase inhibitors)

RN 167683-23-0 HCAPLUS

CN Urea, N-(4-bromo-5-methyl-1H-pyrazol-3-yl)-N'-[2-(2-chloro-3-ethoxy-6-fluorophenyl)cyclopropyl]-, cis- (9CI) (CA INDEX NAME)

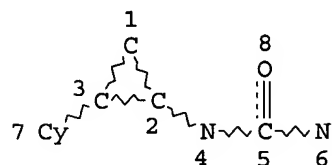
Relative stereochemistry.



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=> d stat que

L1 STR



NODE ATTRIBUTES:

DEFAULT MLEVEL IS ATOM

DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:

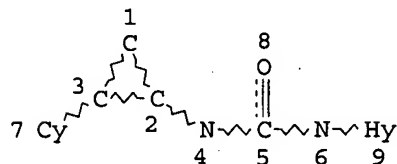
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NUMBER OF NODES IS 8

STEREO ATTRIBUTES: NONE

L3 509 SEA FILE=REGISTRY SSS FUL L1

L4 STR



NODE ATTRIBUTES:

DEFAULT MLEVEL IS ATOM

DEFAULT ECLEVEL IS LIMITED

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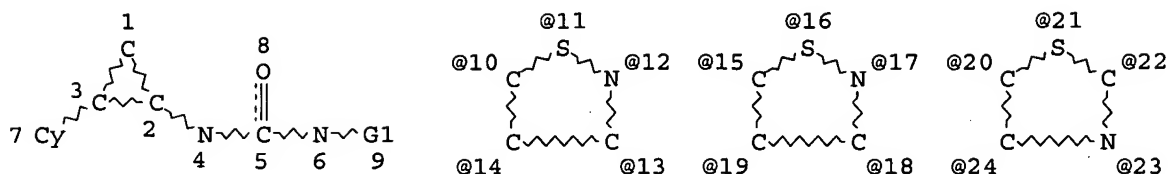
RING(S) ARE ISOLATED OR EMBEDDED

NUMBER OF NODES IS 9

STEREO ATTRIBUTES: NONE

L5 213 SEA FILE=REGISTRY SUB=L3 SSS FUL L4

L10 STR



VAR G1=10/11/12/13/14/15/16/17/18/19/20/21/22/23/24

NODE ATTRIBUTES:

DEFAULT MLEVEL IS ATOM

DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:

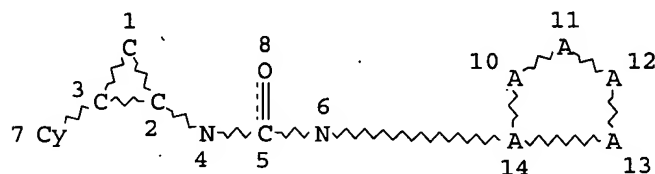
RING(S) ARE ISOLATED OR EMBEDDED

NUMBER OF NODES IS 24

STEREO ATTRIBUTES: NONE

L11 1 SEA FILE=REGISTRY SUB=L5 SSS FUL L10

L12 STR



NODE ATTRIBUTES:

DEFAULT MLEVEL IS ATOM

DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:

RING(S) ARE ISOLATED OR EMBEDDED

NUMBER OF NODES IS 13

STEREO ATTRIBUTES: NONE

L13 18 SEA FILE=REGISTRY SUB=L3 SSS FUL L12

L14 1 SEA FILE=HCAPLUS ABB=ON PLU=ON L11

L15 17 SEA FILE=REGISTRY ABB=ON PLU=ON L13 NOT L11

L16 5 SEA FILE=HCAPLUS ABB=ON PLU=ON L15

L17 5 SEA FILE=HCAPLUS ABB=ON PLU=ON L16 NOT L14

L18 196 SEA FILE=REGISTRY ABB=ON PLU=ON L5 NOT (L11 OR L13)

L19 31 SEA FILE=HCAPLUS ABB=ON PLU=ON L18

L20 30 SEA FILE=HCAPLUS ABB=ON PLU=ON L19 NOT (L14 OR L17)

L21 2 SEA FILE=HCAPLUS ABB=ON PLU=ON L20 AND PD=<AUGUST 24, 1994

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=> d ibib abs hitstr l21 1-2

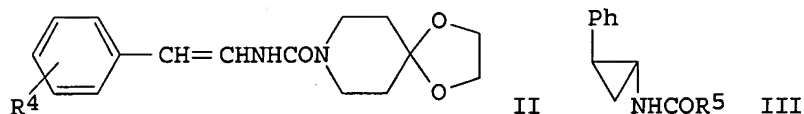
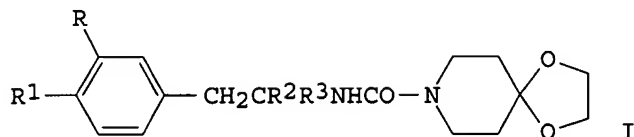
L21 ANSWER 1 OF 2 HCAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 1978:74324 HCAPLUS

DOCUMENT NUMBER: 88:74324

TITLE: Psychoactive agents. IV. Synthesis and CNS depressant activity of some  $\beta$ -arylethyl- and  $\beta$ -styrylureas

AUTHOR(S): Arya, V. P.; David, J.; Grewal, R. S.  
 CORPORATE SOURCE: Ciba-Geigy Res. Cent., Bombay, India  
 SOURCE: Indian Journal of Chemistry, Section B: Organic  
 Chemistry Including Medicinal Chemistry (1977  
 ), 15B(7), 635-40  
 CODEN: IJSBDB; ISSN: 0376-4699  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English  
 OTHER SOURCE(S): CASREACT 88:74324  
 GI



AB Treatment of 3,4-RR1C6H3CH2CR2R3NH2 (R = H, MeO; R1 = H, MeO, Cl, F; R2, R3 = H, Me) with COCl2 gave 3,4-RR1C6H3CH2CR2R3NCO, which reacted with 8-aza-1,4-dioxaspiro[4.5]decane to give the ureas I. Styrylureas II (R4 = H, Cl, F) and (phenylcyclopropyl)ureas III [R5 = Q-Q3, 4-hydroxy-4-(4-fluorophenyl)piperidino, (hexahydroazepin-1-yl)amino, ClCH2CH2CH2NH] were prepared similarly. (Arylethyl)ureas were prepared from 9-aza-3,3-dimethyl-1,5-dioxaspiro[5.5]undecane, 9-aza-1,4-dioxaspiro[4.5]decane, 1-azaspiro[4.5]decane and 3-azaspiro[5.5]undecane. The central nervous system (CNS) depressant and anticonvulsant activity of these compds. were reported.

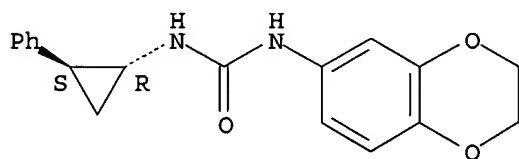
IT 65535-80-0P 65535-81-1P

RL: SPN (Synthetic preparation); PREP (Preparation)  
 (preparation of)

RN 65535-80-0 HCAPLUS

CN Urea, N-(2,3-dihydro-1,4-benzodioxin-6-yl)-N'-(2-phenylcyclopropyl)-, trans- (9CI) (CA INDEX NAME)

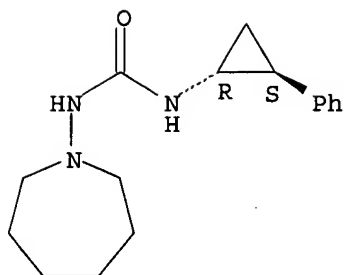
Relative stereochemistry.



RN 65535-81-1 HCAPLUS

CN Urea, N-(hexahydro-1H-azepin-1-yl)-N'-(2-phenylcyclopropyl)-, trans- (9CI)  
 (CA INDEX NAME)

Relative stereochemistry.



L21 ANSWER 2 OF 2 HCAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 1966:468519 HCAPLUS

DOCUMENT NUMBER: 65:68519

ORIGINAL REFERENCE NO.: 65:12792c-e

TITLE: Cytokinin activity of some substituted ureas and thioureas

AUTHOR(S): Bruce, M. I.; Zwar, J. A.

CORPORATE SOURCE: Div. Plant Ind., C.S.I.R.O., Canberra, Australia

SOURCE: Proc. Roy. Soc. (London), Ser. B. (1966), 165(999), 245-65

DOCUMENT TYPE: Journal

LANGUAGE: English

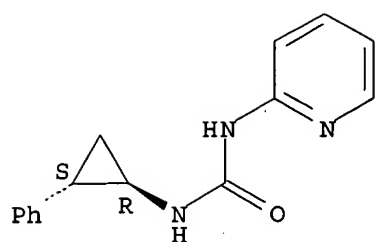
AB N,N'-Diphenylurea had reproducible cytokinin activity. N-Monosubstituted and N,N'-disubstituted ureas (500) were examined, and .apprx.250 were active. The following generalizations were made with regard to the correlation of chemical structure with biol. activity: (1) phenylurea was the simplest active compound; (2) an HNCONH bridge conferred higher activity than an HNCSNH bridge; (3) compds. in which both amino H atoms on 1 or both sides of the bridge were substituted were of low activity or were inactive; (4) ring substitution on the bridge (RNHCONH2, R = substituted phenyl ring) increased the activity, and meta substitutions gave highest activity, while ortho substitutions gave lowest activity; (5) compds. with electron-attracting substituents were more active than those with electron-donating substituents; (6) pyridyl compds. were active, but compds. with non-planar rings were inactive; and (7) in compds. of the type RNHCONHR', where R and R' were phenyl or substituted phenyl groups, compds. having 1 unsubstituted phenyl ring had higher activities than those having 2 substituted phenyl groups. Some ureas showed detectable activity at 0.1 ppm., which was .apprx.4-fold less active than kinetin in the tobacco pith assay.

IT 13257-07-3, Urea, 1-(2-phenylcyclopropyl)-3-(2-pyridyl)-, trans- (plant regulator activity of)

RN 13257-07-3 HCAPLUS

CN Urea, 1-(2-phenylcyclopropyl)-3-(2-pyridyl)-, trans- (8CI) (CA INDEX NAME)

Relative stereochemistry.



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